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BICRYSTALS WITH STRAIN GRADIENT EFFECTS

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ABSTRACT

The boundary between two perfectly bonded single crystals plays a very important role in determining the deformation of the bicrystal. This work addresses the role of the grain boundary by considering the elevated hardening of a slip system due to a slip gradient. The slip gradients are associated with geometrically necessary dislocations and their effects become pronounced when a representative length scale of the deformation field is comparable to the dominant microstructural length scale of a material. A new rate-dependent crystal plasticity theory is presented and has been implemented within the finite element method framework. A planar bicrystal under uniform in-plane loading is studied using the new crystal theory. The strain is found to be continuous but non-uniform within a boundary layer around the interface. The lattice rotation is also non-uniform within the boundary layer. The width of the layer is determined by the misorientation of the grains, the hardening behavior of slip systems, and most importantly by the characteristic material length scales. The overall yield strength of the bicrystal is also obtained. A significant grain-size dependence of the yield strength, the Hall-Petch effect, is predicted.

INTRODUCTION

Conventional continuum mechanics theories assume that stress at a material point is a function of state variables, primarily strain, at the same point only. This *local* assumption has long been proved to be adequate when the wave length of a deformation field is much larger than the dominant length scale of its micro-structure. However, when the two length scales are comparable, the assumption is questionable as the material behavior at a point is influenced by the deformation at neighboring points. Various *non-local* or *strain gradient* continuum theories have been proposed to model material deformation more accurately when local theories may be inadequate, notably [1-5]. Among them [1-2] were developed for linear elastic materials while [3-5] are for plastic deformation.

Although there have been a considerable number of publications on strain gradient theories, most of them deal with phenomenological theories for homogenized polycrystals. A new crystal plasticity theory with strain gradient effects has been proposed [5]. The theory considers the hardening effects due to both slip and slip gradients. The new crystal theory is applied to study the grain-size effect of yield strength of a polycrystal [6]. In the theory, the slip and slip gradients are related to the macroscopic strain and strain gradients and the slip gradients are indeed the spatial derivatives of slip. This treatment, although valid in [6] for the special constitutive law used, needs to be modified for a crystal having an incremental constitutive law. In [7], a new notion is introduced for the slip gradients. It is based on a homogenization process of the crystal at two different length scales, i.e., a macro scale at which a strain gradient theory applies and a micro scale at which the material exhibits no strain gradient effects. Homogenization suggests that a slip gradient in the constitutive law for a macroscopic material point is the gradient of slip at the microscale, and it generally differs from the slip gradient at the macro scale. Adopting this notion, a modified strain gradient crystal plasticity theory has been established in [7] based on the same basic assumptions in [5-6].

A new finite element code, GRACY2D, has been developed for the modified strain gradient crystal theory and is applied here to study the infinitesimally small deformation of a planar bicrystal under in-plane loading. Attention is focused on the deformation around the grain boundary and on the grain size effect on the overall yield strength of the bicrystal, the well-known Hall-Petch effect.

RATE-DEPENDENT STRAIN GRADIENT CRYSTAL PLASTICITY THEORY

In this section, a formulation of rate-dependent strain gradient crystal plasticity theory is presented. The formulation is based on an alternative theory proposed by [5] and applied in a study of the Hall-Petch effect [6]. A material point of a strain gradient theory solid can sustain Cauchy stress σ_{ij} and *double stress* τ_{ijk}. Deformation is characterized by strain $\varepsilon_{ij} = (u_{i,j} + u_{j,i})/2$ and strain gradient $\eta_{ijk} = u_{k,ij}$. Here a subscript comma indicates a partial derivative with respect to a Cartesian coordinate. A principle of virtual work has been given in [2, 5] and will not be repeated here for briefness of the presentation. The plastic part (indicated by a superscript p) of macroscopic strain rate is related to the crystal slip rate through

$$\dot{\varepsilon}^p_{ij} = \sum_\alpha \dot{\gamma}^{(\alpha)} \mu^{(\alpha)}_{ij}, \qquad \mu^{(\alpha)}_{ij} = \frac{1}{2}\left(s^{(\alpha)}_i m^{(\alpha)}_j + s^{(\alpha)}_j m^{(\alpha)}_i\right) \tag{1}$$

where $\dot{\gamma}^{(\alpha)}$ is the slip rate on slip system α. Here $\mathbf{s}^{(\alpha)}$ and $\mathbf{m}^{(\alpha)}$ are the unit vectors in the slip direction and slip plane normal direction of the α-th slip system respectively. (A third unit vector $\mathbf{t}^{(\alpha)} = \mathbf{s}^{(\alpha)} \times \mathbf{m}^{(\alpha)}$ is the transverse direction.) Similarly,

$$\dot{\eta}^p_{ijk} = \sum_\alpha \dot{\gamma}^{(\alpha)}_r \psi^{(\alpha)}_{rijk}, \quad \psi^{(\alpha)}_{rijk} = \delta_{ri} s^{(\alpha)}_k m^{(\alpha)}_j + \delta_{rj} s^{(\alpha)}_i m^{(\alpha)}_k - \delta_{rk} s^{(\alpha)}_i m^{(\alpha)}_j + \frac{1}{2} t^{(\alpha)}_r e_{ijk} \tag{2}$$

where $\dot{\gamma}^{(\alpha)}_r$ is the micro slip rate gradient in the r-th Cartesian coordinate axis direction [7]. We denote the micro slip rate gradients in the directions $\mathbf{s}^{(\alpha)}$, $\mathbf{m}^{(\alpha)}$ and $\mathbf{t}^{(\alpha)}$ as $\dot{\gamma}^{(\alpha)}_s$, $\dot{\gamma}^{(\alpha)}_m$ and $\dot{\gamma}^{(\alpha)}_t$ respectively. The work conjugates of the micro slip rate gradients along these crystallographic directions are denoted as $Q^{(\alpha)}_s$, $Q^{(\alpha)}_m$ and $Q^{(\alpha)}_t$ respectively. As in [5-6], slip of crystallographic system is assumed to depend on a scalar *effective* shear stress defined as

$$\tau^{(\alpha)}_e = \left((\tau^{(\alpha)})^2 + (\ell_s^{-1} Q^{(\alpha)}_s)^2 + (\ell_m^{-1} Q^{(\alpha)}_m)^2 + (\ell_t^{-1} Q^{(\alpha)}_t)^2\right)^{1/2} \tag{3}$$

where ℓ_s, ℓ_m and ℓ_t are three constitutive length scales. Plastic flow of a slip system obeys the following normality rule:

$$\dot{\gamma}^{(\alpha)} = \dot{\gamma}^{(\alpha)}_e \frac{\tau^{(\alpha)}}{\tau^{(\alpha)}_e}, \quad \ell_s \dot{\gamma}^{(\alpha)}_s = \dot{\gamma}^{(\alpha)}_e \frac{\ell_s^{-1} Q^{(\alpha)}_s}{\tau^{(\alpha)}_e}, \quad \ell_m \dot{\gamma}^{(\alpha)}_m = \dot{\gamma}^{(\alpha)}_e \frac{\ell_m^{-1} Q^{(\alpha)}_m}{\tau^{(\alpha)}_e}, \quad \ell_t \dot{\gamma}^{(\alpha)}_t = \dot{\gamma}^{(\alpha)}_e \frac{\ell_t^{-1} Q^{(\alpha)}_t}{\tau^{(\alpha)}_e} \tag{4}$$

where

$$\dot{\gamma}^{(\alpha)}_e = \left((\dot{\gamma}^{(\alpha)})^2 + (\ell_s \dot{\gamma}^{(\alpha)}_s)^2 + (\ell_m \dot{\gamma}^{(\alpha)}_m)^2 + (\ell_t \dot{\gamma}^{(\alpha)}_t)^2\right)^{1/2}. \tag{5}$$

In this paper, a power-law creep model is assumed for the effective slip rate:

$$\dot{\gamma}^{(\alpha)}_e = \dot{\gamma}_0 \left(\frac{\tau^{(\alpha)}_e}{g^{(\alpha)}}\right)^{1/n} \tag{6}$$

where n is the rate-dependence index, $\dot{\gamma}_0$ a reference slip rate and $g^{(\alpha)}$ the hardness of slip system α. In the unloaded state all slip systems have the same initial hardness of τ_0. Slip systems harden according to the following hardening law:

$$\dot{g}^{(\alpha)} = \sum_{\beta} h_{\alpha\beta}\dot{\gamma}_c^{(\beta)}, \qquad h_{\alpha\beta} = h\delta_{\alpha\beta} + qh(1-\delta_{\alpha\beta}). \tag{7}$$

Here q is a constant latent hardening index. The self-hardening modulus, h, is assumed to be a constant. The hardening law (7) reflects the elevated hardening due to geometrically necessary dislocations whose density is proportional to the slip gradients [5]. In [5-6], $\dot{\gamma}_r^{(\alpha)}$ is identified as the macro slip rate gradient $\dot{\gamma}_{,r}^{(\alpha)}$. This imposes extra kinematic constraints which would generally contradict the normality rule (Eqn.(4)). Based on a homogenization process of the crystal behavior at two length scales, $\dot{\gamma}_r^{(\alpha)}$ should be interpreted as the micro slip rate gradient and is generally different from $\dot{\gamma}_{,r}^{(\alpha)}$ [7].

To complete the formulation, an elasticity constitutive law must be specified. All the computations reported in this paper are obtained using the following elasticity constitutive law:

$$\dot{\sigma}_{ij} = \frac{E}{1+\nu}\left(\dot{\varepsilon}_{ij}^e + \frac{1}{1-2\nu}\dot{\varepsilon}_{kk}^e\delta_{ij}\right), \qquad \dot{\tau}_{ijk} = 2E\ell^2\dot{\eta}_{ijk}^e \tag{8}$$

where E and ν are the Young's modulus and Poisson's ratio of the crystal. Elastic anisotropy is neglected. ℓ is an internal length scale which is assumed to be a material parameter.

The above rate-dependent strain gradient crystal theory has been implemented within the finite element method framework. A new finite element code, GRACY2D, is developed for the special case of crystals undergoing a plane deformation. The details of the finite element implementation are presented in [8].

RESULTS

As an application of the strain gradient crystal plasticity theory, a bicrystal under plane strain conditions is studied. As schematically shown in Fig.1, the bicrystal consists of two perfectly bonded single crystal grains infinitely long in the x_1- direction and of a height of D in the x_2-direction. The two grains are cut from the same single crystal but are misaligned during bonding. Each grain is assumed to have only two slip systems. The slip direction and the slip plane normal direction of each slip system are both in the plane. The bicrystal is loaded by a uniformly prescribed velocity $\dot{u}_1^*$ along the top surface while the bottom surface is perfectly gripped. Along

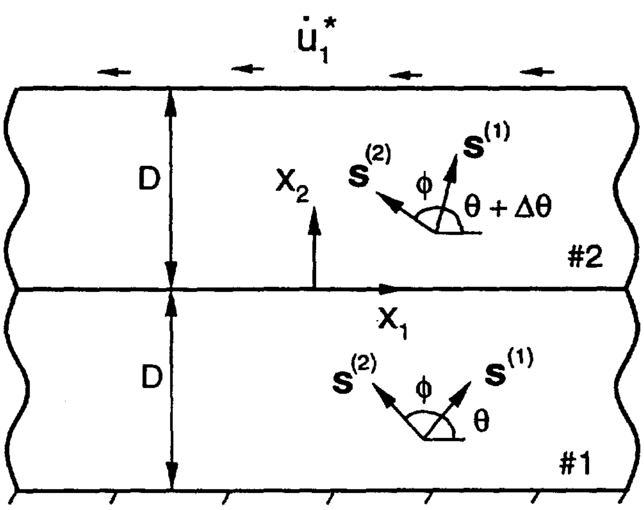

Figure 1. Schematic illustration of a planar bicrystal under in-plane loading

both surfaces there are no double stress tractions. The slip directions of the two slip systems in grain #1 are set at 30° and -30° with respect to the x_2- axis to limit the number of variables in the problem. All the results presented below are calculated using the following parameters: the average shear strain rate $\dot{\bar{\varepsilon}}_{12} = \dot{u}_1^* / 2D$ is set at 10^{-3} per second, $E = 10^3 \times \tau_0$, $\nu = 0.25$, $\dot{\gamma}_0 = 10^{-3} s^{-1}$, $h = 10 \times \tau_0$, and $n = 0.01$ to approximate the limiting case of a rate-independent bicrystal. The elastic length scale ℓ and the three plastic length scales, ℓ_s, ℓ_m and ℓ_t, are taken to be identical.

The uniformity of the boundary conditions in the x_1- direction dictates that the deformation is also uniform in the direction. The finite element mesh for the computations reported in this paper is drawn on a rectangular portion of the bicrystal 'cut' along the x_3- direction. The width of the rectangle in the x_1- direction is 0.5ℓ and fixed for all computations. Periodic boundary conditions are applied on the left and right hand-side surfaces of the mesh to mimic the uniformity of deformation in the x_1- direction.

Boundary Layer of Non-uniform Deformation

First consider a bicrystal of two large grains with $D = 100\ell$. Conventional crystal plasticity theory predicts that shear stress is uniform throughout the whole structure in order to satisfy equilibrium both in the body and on the surface. Substitution of the uniform shear stress into crystal constitutive law leads to strain and lattice rotation distributions which are uniform in each grain but discontinuous across the grain boundary. This is associated with the discontinuity in the initial lattice orientation. The inclusion of strain gradient effects changes the deformation field significantly near the grain boundary. The total shear strain ε_{12} has a non-uniform but continuous distribution across the grain boundary; away from the grain boundary, the strain approaches the conventional crystal theory predictions. The trend of ε_{12} is broadly similar to that shown in [4] for a phenomenological strain gradient theory solid and therefore will not be presented here. The slip direction of each slip system rotates by

$$\omega = \varepsilon_{12} \cos 2\theta + (\varepsilon_{22} - \varepsilon_{11}) \sin\theta \cos\theta + \omega^e \tag{9}$$

where ω^e is the elastic rotation angle of the material and is given by

$$\omega^e = (\partial u_2 / \partial x_1 - \partial u_1 / \partial x_2)/2 + \sum_{\alpha} \gamma^{(\alpha)} / 2. \tag{10}$$

The rotation of slip system (2) is plotted in Fig. 2 in which the lattice of grain #2 is misaligned by

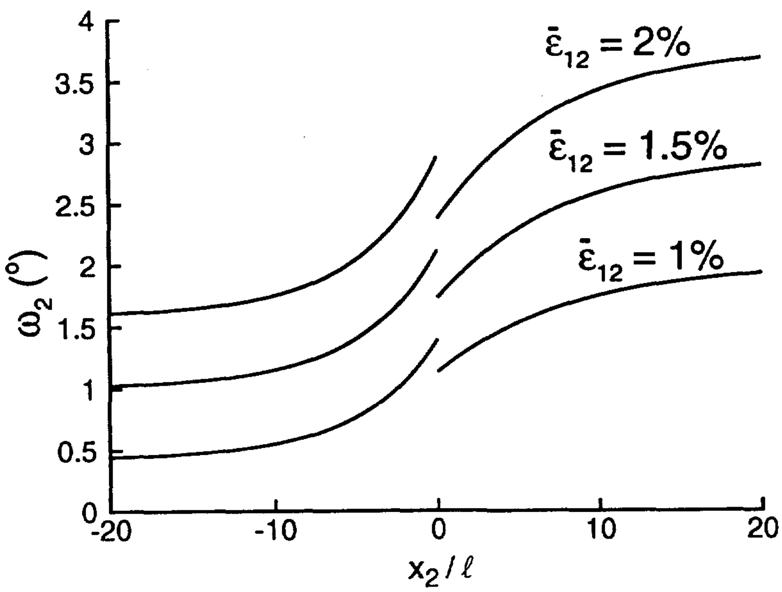

Figure 2. Distribution of the rotation angle of the second slip plane

20° counterclockwise from that of grain #1. The rotation has a non-uniform distribution around the boundary. Similar distributions are found for the material elastic rotation and rotation of slip system (1). It is interesting to note that grain #1 rotates by a larger angle than grain #2 around the interface. This suggests that the grains deform to accommodate each other, in that the mismatch of the lattice orientations is reduced, though by a small amount. It remains to see to what extent the lattice mismatch can be reduced at a finite deformation. It is worth pointing out that the conventional theory predicts that the mismatch will be enhanced as indicated by the rotations away from the interface. The rotation of slip plane (1) and the material elastic rotation have broadly similarly distributions and therefore are not shown here.

In the strain gradient crystal theory, there are several length scales which are assumed to be identical in the current problem. Because the width of the boundary layer is a function of the bicrystal properties, e.g. lattice mismatch and the constitutive length scale ℓ, the correlation between numerical calculation and experimental measurement of lattice rotation provides a means of determining ℓ. Fig.3 shows the boundary layer width in the second grain, normalized by ℓ, as a function of the lattice mismatch angle $\Delta\theta$. The boundary layer width is chosen to be the distance from the grain boundary at which the material elastic rotation angle differs by 0.2° from that remote from the interface and it increases with overall straining. It is observed that when the mismatch angle is close to 30°, the layer width in grain #2 has a peak. Recall that the slip directions of grain #1 are set at 30° and -30°, at a mis-match of 30°, grain #2 has one slip system with a Schmid factor of 1.0, is therefore more compliant, undertakes a larger portion of the overall deformation and has a more extended boundary layer. At 60° mismatch, grain #2 has one slip plane perpendicular to x_2- direction, therefore little material elastic rotation is needed.

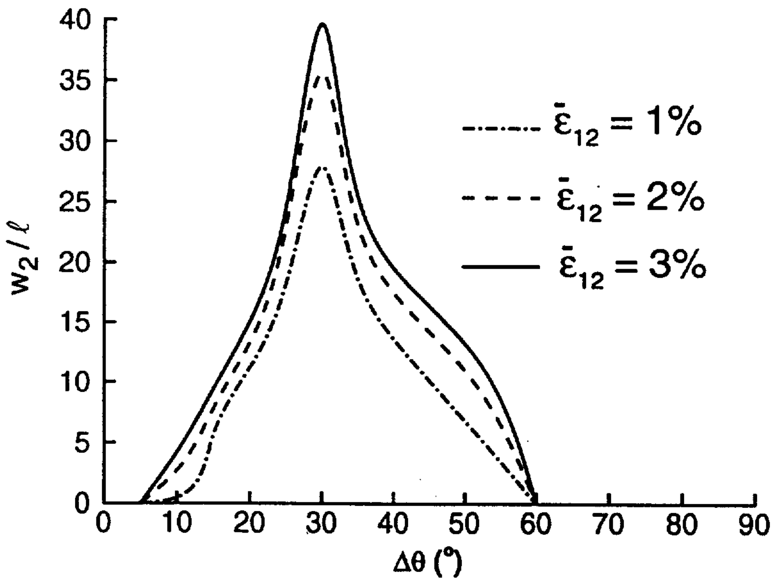

Figure 3. Width of the boundary layer in Grain #2 as a function of lattice mismatch angle

Hall - Petch Effect

It is well known that the yield strength of a polycrystal scales as the inverse square root of the grain size in the material. This is the so-called Hall-Petch Effect. Due to the lack of any constitutive length scales, a conventional crystal plasticity theory fails to predict the Hall-Petch effect. The grain size-dependence of the overall shear yield strength of the bicrystal shown in Fig. 1 is studied using the current strain gradient crystal theory. The overall 'yield strength' of the bicrystal τ_y is defined as the surface traction per unit area at 0.1% plastic average strain. τ_y is plotted in Fig.4 versus grain size D for various lattice mismatch. It can be seen that the grain size effect diminishes as D exceeds about 100ℓ. The yield strength increases significantly as D is decreased. The Hall-Petch effect is most significant when the lattice mismatch is large, and it completely disappears when there is no mismatch. A vanishing mismatch leads to no strain gradients, hence to no size-dependence of the yield strength.

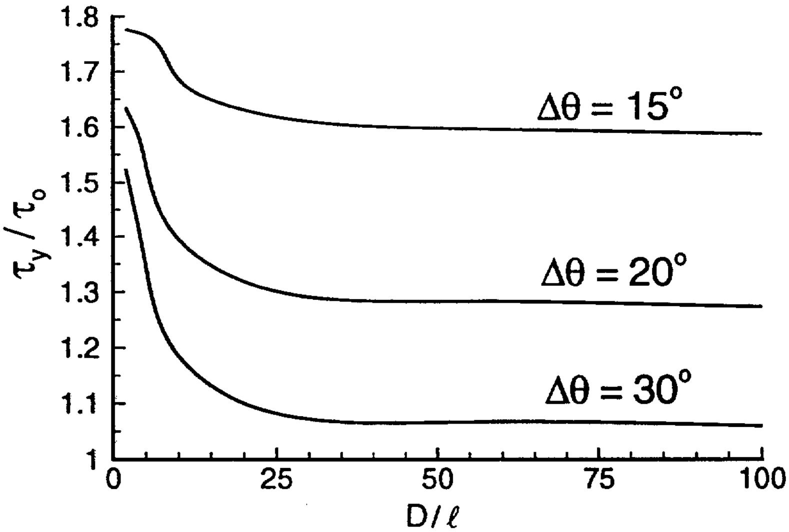

Figure 4. The grain size-dependence of the overall yield strength of the bicrystal

CONCLUSIONS

A rate-dependent crystal plasticity theory with strain gradient effects is presented. It is based on the physical notion of elevated strain hardening of slip systems due to geometrically necessary dislocations. The new crystal theory is implemented within the finite element framework and is used to study the deformation of a planar bicrystal under uniform in-plane loading. The strain and crystal rotation are found to be non-uniform within a boundary layer. The boundary layer width is determined by the grain boundary characteristics, such as lattice mismatch, and the material constitutive length scales. The overall yield strength of the bicrystal is found to depend on the size of the grains. The size effect is significant for a bicrystal with a large lattice mismatch.

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